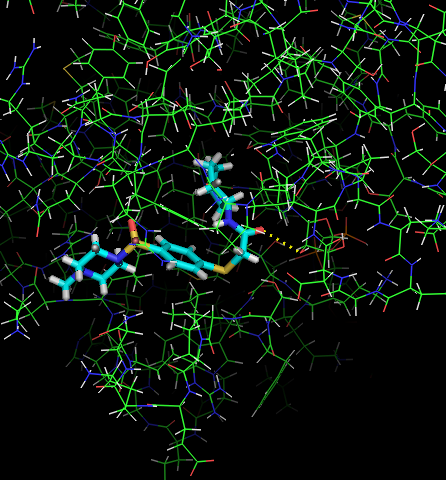
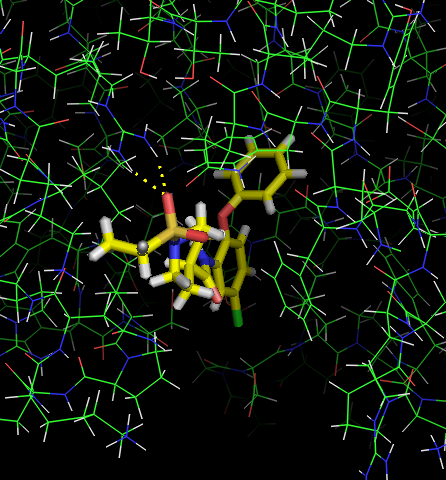
1. Top 10 ligands



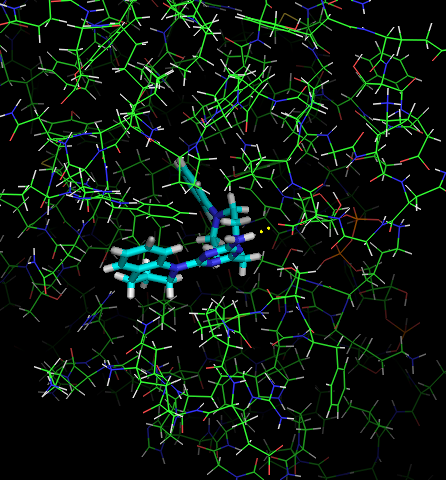
1. Pictures of top 10 ligands with their polar contacts with original ligand
2. 9036564: 1 polar contact



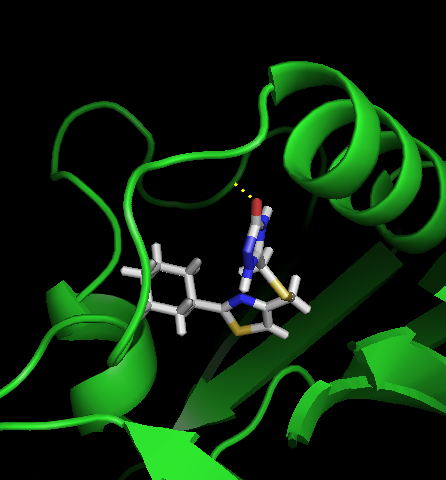
1. 9057940: 2 polar contacts



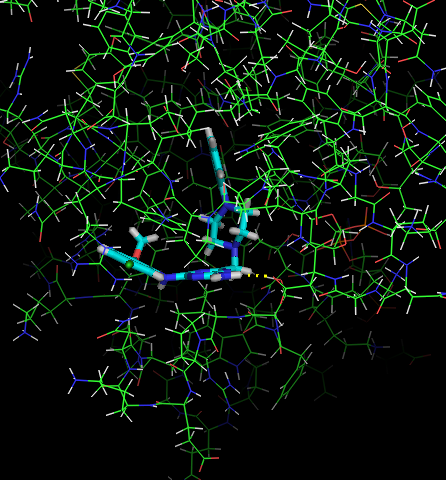
1. 9039798: 1 polar contact



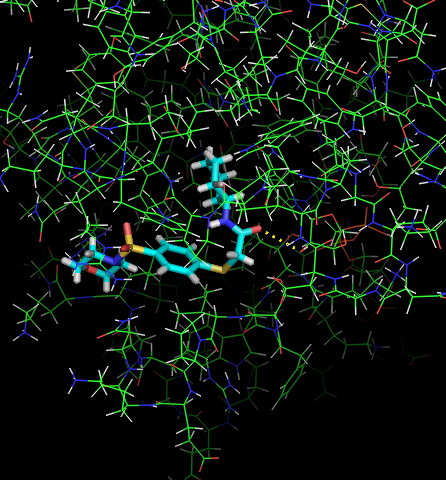
1. 9040519: 1 polar contact



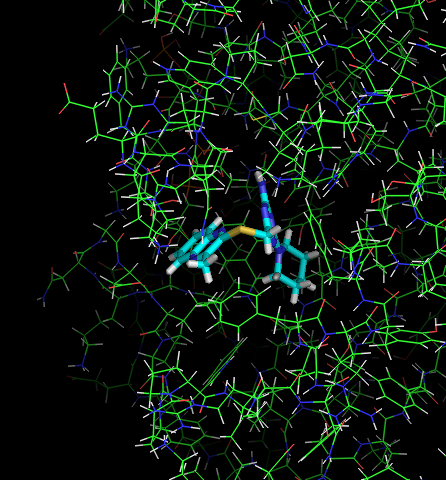
1. 9037146: 1 polar contact



1. 9038483: 1 polar contact



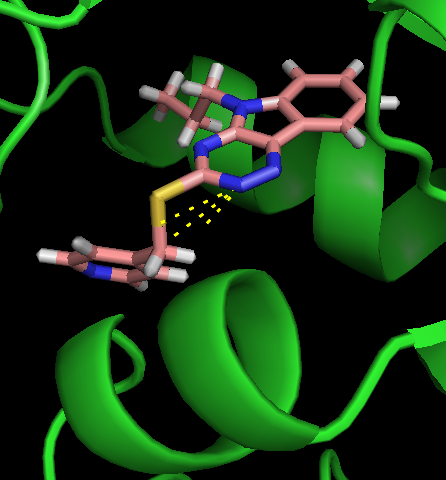
1. 9038770: no polar contact



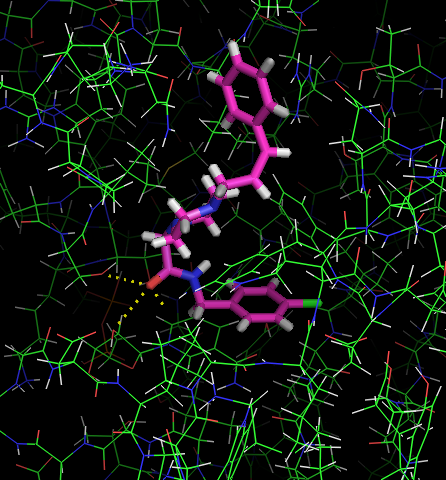
1. 9061456: 4 polar contacts



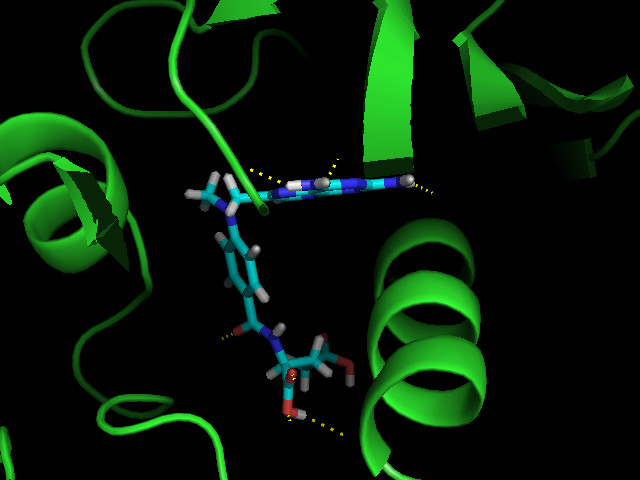
1. 9067226: 3 polar contacts



1. 9049544: 3 polar contacts



1. Polar contact between original ligand and MTX extracted: there are 7 polar contacts



1. Properties of top 3 ligands

|  |  |  |
| --- | --- | --- |
| 1 | 2 | 3 |
| **# 9036564** | **# 9057940** | **# 9039798** |
| |  | | --- | |  | |  |  |
| Formula | Formula | Formula |
| *C19 H29 N3 O3 S2* | *C20 H23 Cl N2 O4 S* | *C23 H26 F N7* |
| Molecular Weight | Molecular Weight | Molecular Weight |
| *412* | *423* | *420* |
| LogP | LogP | LogP |
| *3.09* | *3.43* | *3.74* |
| LogSW | LogSW | LogSW |
| *-4.84* | *-4.8* | *-4.44* |
| Rotatable Bonds | Rotatable Bonds | Rotatable Bonds |
| *5* | *4* | *4* |
| Hdon | Hdon | Hdon |
| *1* | *1* | *1* |
| Hacc | Hacc | Hacc |
| *5* | *5* | *4* |